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Electronic Properties of Carbon at Extreme Conditions from ab Initio Simulations

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March 30, 2004

2004 March American Physical Society Meeting
Montreal, Canada
March 22, 2004 through March 26, 2004

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Electronic properties of Carbon at extreme conditions from ab initio simulations

A. A. Correa^{1,2} S. A. Bonev² G. Galli² R. W. Falcone¹

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APS March meeting, Montreal 2004



Why Carbon at extreme conditions?

- **Astrophysics and Planetary Science:** Jovian Planets¹ and White Dwarfs²
- **Technology:** High-pressure research, transparency problem³

Why *ab initio* simulation?

- **Practical:** Experiments are difficult at extreme conditions and results are controversial.
- **Methodology:** Empirical/non-*ab initio* simulations gave misleading results⁴.

Electronic Gap dependence with Pressure and Temperature

¹W. B. Hubbard, *Science* **214**, 145-9 (1981)

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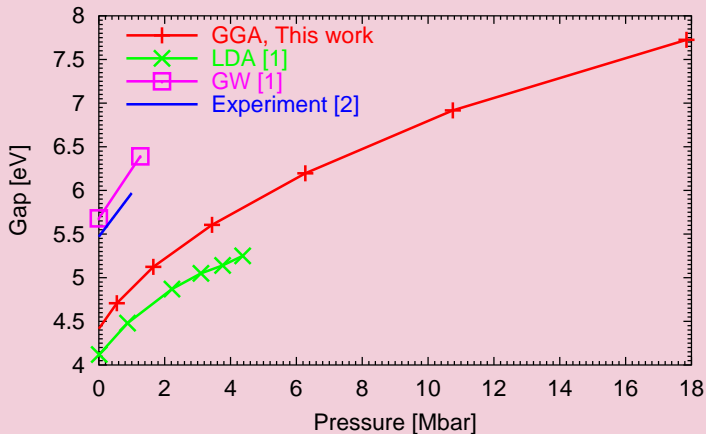
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Gap of Diamond increases with Pressure

Gap dependence with Pressure at $T = 0$, Unusual opening of the Gap



[1] Surh et al., PRB 45,8239 (1992)

[2] Dean et al., PRA 140,355 (1965)



Gap Increase with Pressure is determined by Two Factors

1. sp^3 hybridization

- Simple **Bonding-Antibonding picture** works for diamond⁵.
- **Silicon** shows opposite behaviour.

2. Symmetry of Diamond structure

- Under **Anisotropic pressure** the gap decreases.
- **BC8** shows a decrease of the gap.
- **Thermal disorder** produces a rapid decrease of the gap.

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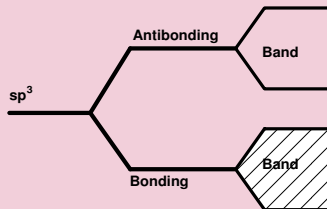
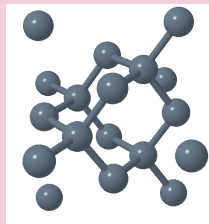
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Diamond, Formation of bands



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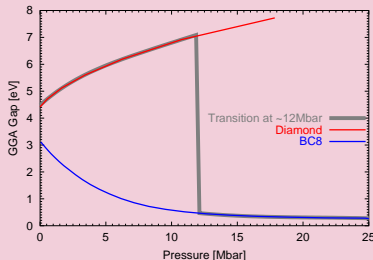
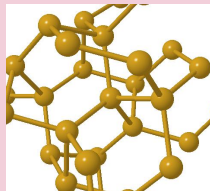
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BC8 structure, stable above 12Mbar



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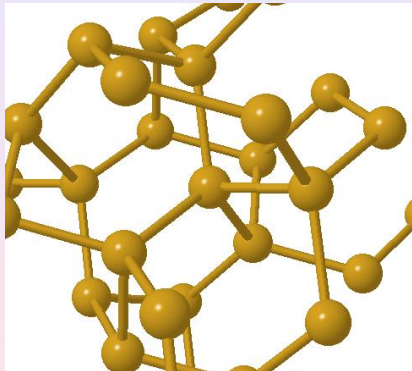
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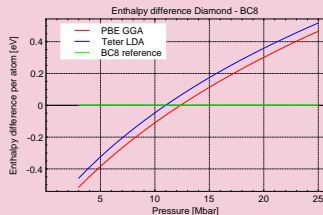
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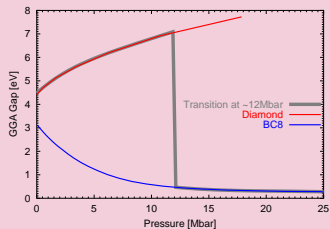
BC8 Structure, 4-fold coord. but different to Diamond



Stable above 12 Mbar, ΔH method



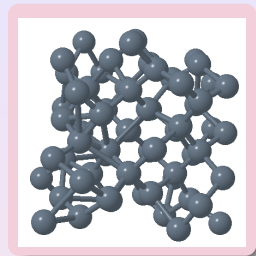
BC8 Gap decreases with Pressure



Gap of Diamond at Finite Temperature: Method

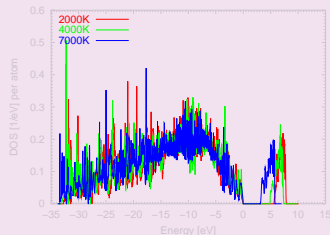
Constant Pressure Molecular Dynamics

- **64 atoms** in a periodic box
- **Car-Parinello** molecular dynamics
- **Norm conserving** pseudo-potential
- Set $P = \sim 10\text{Mbar}$ and $T = 0$ up to 10000K
- ~ 4 picoseconds **equilibration** time



Density of States

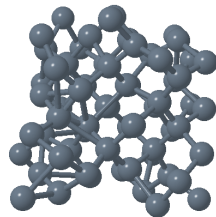
- **DOS** calculated from **Snapshots**
- GGA Energy **Gap** from DOS.



Gap of Diamond at Finite Temperature: Method

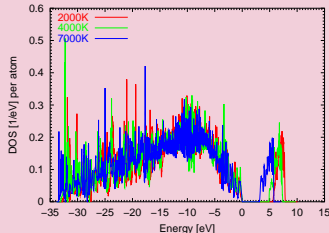
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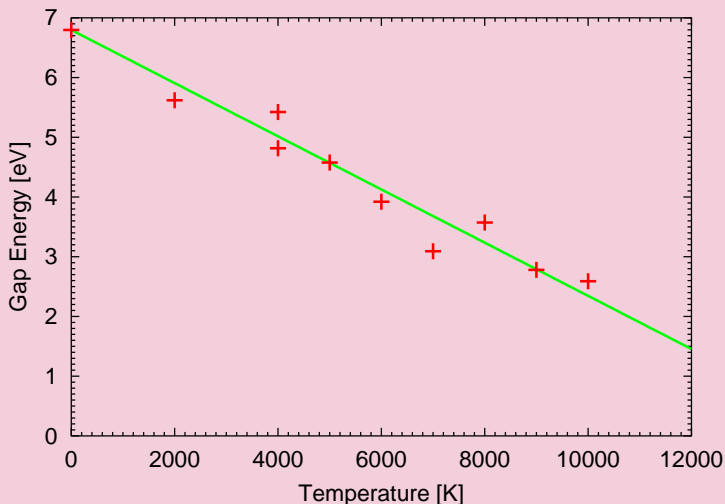
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Gap of Diamond reduces with Temperature at High P

Gap dependence with Temperature at $P = 10$ Mbar



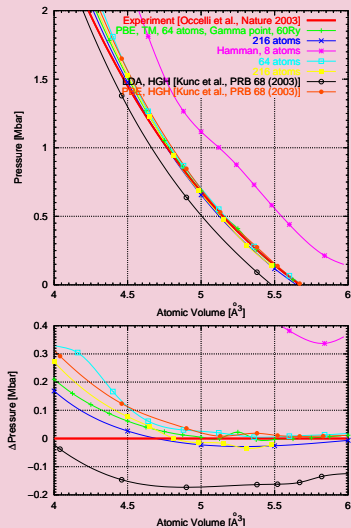
Summary

- Energy Gap of Carbon is very sensitive to crystal symmetry.
- BC8 Gap decreases with pressure.
- Diamond Gap increases with pressure.
- but decreases continuously as temperature is raised.
- Diamond at High pressure does not become conducting before melting

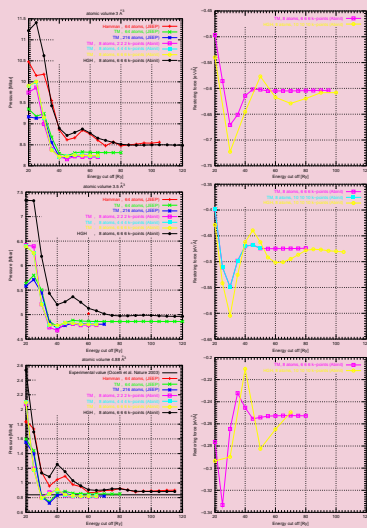


Appendix: Convergence tests

Equation of State at $T = 0$, size FX



EOS and forces: Energy cut-off FX



This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.